Whence the odd-even staggering in nuclear binding?

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We explore the systematics of odd-even mass staggering with a view to identifying the physical mechanisms responsible. The BCS pairing and mean field contributions have A- and number parity dependencies which can help disentangle the different contributions. This motivates the two-term parametrization c_1+c_2/A as a theoretically based alternative to the inverse power form traditionally used to fit odd-even mass differences. Assuming that the A-dependence of the BCS pairing is weak, we find that mean-field contributions are dominant below mass number $A \sim 40$ while BCS pairing dominates in heavier nuclei.

I. INTRODUCTION

The observed odd-even mass staggering has been extensively explored in the literature[1, 2, 3, 4, 5] The effect has generally been associated with the pairing gap Δ, as suggested by BCS theory. When examined over the full table of measured nuclides [6], the values for the staggering display a great deal of scatter. However, a slow trend with nuclear mass number A is also observed. This trend has been extensively analyzed in the literature by fitting data to an inverse power of A. Traditionally this has been $1/A^{1/2}$, but other powers are used as well[4, 7, 8]. For example, ref. [4] advocates an expansion in powers of $A^{-1/3}$, based on the finite-size analysis in ref. [17]. There is no theoretical justification for a single-term fractional-power dependence, however.

It has been suggested that, in addition to the anticipated BCS type of pairing,

other effects contribute significantly to the staggering [1, 3, 5]. One would anticipate that each contribution would have its own characteristic dependence on A. Consequently the staggering should follow some combination of these. The tradition of representing the net effect by a form with a single fractional exponent obscures the complexity of the effect. We propose here a different form that may offer a better opportunity to identify the various contributing effects.

There are a number of difference formulas that may be used as measures for the staggering[7, 9, 10]. In this work we use the measure conventionally called $\Delta^{(3)}$ [1, 3, 4]. It involves the difference between the two separation energies of adjacent nuclei. Here the removal of one type of nucleon, i.e., proton or neutron, is considered, while the number of the opposite isospin is kept the same. We believe it is the most direct measure of staggering and is the most convenient quantity for theoretical study. One defines the *neutron OES* as

$$\Delta^{(3)}_{on}(N,Z)) = -(-)^{\pi_N}\frac{1}{2}\left(S_n(N+1,Z) - S_n(N,Z)\right) \tag{1}$$

Here S_n is the separation energy, $S_n(N) = B(N)-B(N-1)$ and B the binding energy. The factor depending on the number parity π_N is chosen so that the OES centered on even and odd neutron numbers N will both be positive for normal attractive pairing. The proton OES are defined similarly and we designate them by $\Delta^{(3)}_{op}$ and $\Delta^{(3)}_{ep}$.

The 4-point measure used by Bohr and Mottelson [9, Eqs. 2-92, 2-93] is the average of adjacent even and odd values of $\Delta^{(3)}$. We will also find it convenient to examine the average and differences of our parametrized OES, but that does not require contiguous data. It should also be noted that, because the $\Delta^{(3)}$ values represent second differences of the binding energies, they may be non-zero even without any odd-even staggering.

The various OES offer interesting possibilities for examining the various contributions. First, the even and odd OES have different contributions that can possibly be distinguished. Second, the two isospins (neutron and proton) can be compared to give some indication of the role of the Coulomb and other isospin dependent effects.

II. MECHANISMS

There are a several mechanisms that contribute to OES in framework of mean field theory. We consider three of them: single-particle energies, BCS pairing, and orbital interaction energies. We will assume that orbitals are two-fold degenerate between time-reversed partner states to estimate single-particle and diagonal interaction energies. A summary of the following discussion is provided in Table I below, which lists separately the contributions pertinent to $\Delta^{(3)}_o$ and $\Delta^{(3)}_e$. There are several kinds of orbital interaction that affect the systematics of the OES. Most important are the spin- and symmetry-dependent interactions that are classified under "time-odd fields" in the density functional formulation of mean-field theory. But also the Coulomb interaction and the ordinary isospin-spin dependent interactions play a role when examining the differences of $\Delta^{(3)}$ measures. Another mechanism that has been suggested [1, 3] involves the static polarization of the core by the valence orbitals. However, it has no obvious parametric dependence on A, and we must assume that its contribution is small to carry out

the present analysis.

TABLE I: Contributions to odd-even staggering of nuclear binding energies, and their assumed A-dependence.

Mechanism	$\Delta_o^{(3)}$	$\Delta_e^{(3)}$	A-dependence
Single-particle	0	$(e_i - e_{i-i})/2$	$1/A$
BCS correlation	Δ_{BCS}	Δ_{BCS}	const.
time-odd	$-v_{i\bar{i},i\bar{i}}/2$	$\bar{v} - v_{i\bar{i},i\bar{i}}/2$	$1/A$

A. Single-particle energies

This mechanism is discussed in many places, e.g., ref. [1], and we repeat the argument for completeness. The binding energy associated with the single-particle Hamiltonian is the negative of the eigenvalue e_i. The neutron (or proton) orbitals are doubly degenerate implying that the contribution from the two separation energies odd OES. On the other hand, the two separation energies in the even OES come from different orbitals. The resulting OES are

$$\Delta_o^{(3)}(s.p.) = 0; \quad \Delta_e^{(3)}(s.p.) = (e_i - e_{i-1})/2. \qquad (2)$$

For brevity we will refer to this as the "single-particle" contribution. The average difference in single-particle energies can be estimated in the Fermi gas model as [9]

$$e_i - e_{i-1} \approx 4e_F/3N \approx 93/A, \text{ MeV}. \qquad (3)$$

In the last approximate equality we have estimated the level spacing using $e_F \approx 35$ MeV and $A \approx 2N$.

B. BCS correlation energy

To avoid confusing the BCS correlation energy with the mean-field energies, let us define it as the additional energy associated with an interaction of the form

$$\sum_{i\neq j}{}' v_{i\bar{i},j\bar{j}} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j. \qquad (4)$$

The orbital $\bar{i}$ is the time-reversed partner of orbital i. The prime on the summation indicates that a sum over i takes only one member of the partners $(i, \bar{i})$. The restriction to $i \neq j$ ensures that there is no mean-field contribution. In the large number limit, the BCS energies give the familiar result, $\Delta_{o,e}^{(3)} = \Delta_{BCS}$, where Δ_{BCS} is the pairing condensate energy for an orbital at the Fermi surface. We will refer to this contribution as the "pairing" contribution.

The A-dependence of the BCS pairing is an open question at present. An analytic treatment can be carried out[17] following the derivation of the BCS formula,

$$\Delta(BCS) = 2Se^{-1/(G\rho(\mu))}. \qquad (5)$$

Here S is the half-width of the truncation zone, G is an average pairing interaction matrix element and $\rho(\mu)$ is the density of levels at the Fermi-energy, μ. For large A, we have $G \sim 1/A$ and $\rho \sim A$ giving a constant Δ. At the next order in a finite-size expansion both G and ρ add terms varying as $A^{-1/3}$. This gives an overall A-dependence $\Delta(BCS) \sim \exp(c/A^{1/3})$ [17]. However, the finite range of the nuclear interaction as well as the induced pairing introduces additional A dependencies that are hard to estimate. In a recent global study [18] it was found that the A dependence of the average OES is quite weak, taking pairing interactions with density dependence as commonly used. We shall therefore make the simplest assumption here, that the BCS correlation energy contribution is independent of A. Finally, we note that although Eq. (2) was derived only for the Hartree-Fock limit, it remains approximately valid in the presence of the pairing Hamiltonian Eq. (4).

C. Time-odd fields

A semi-analytic treatment of this mechanism is given in ref. [11]. There it is called a polarization effect, but in fact it is present in the diagonal orbital interaction. The expressions for the effect are quite different depending on whether one is using a density functional formalism or a formalism based on interaction matrix elements between orbitals. The first formalism has unphysical self-energies that are canceled by the exchange term in the interaction. In the second formalism self-interactions do not appear and one does not make use of single-particle fields and their transformation properties under time reversal. For simplicity in the following we follow the approach based on interaction matrix elements. In this formulation, we count the interactions as particles are added to the system, always filling both orbitals of a Kramers pair if possible. Suppose we start with an even-even system with A nucleons and add another neutron in orbital i. The additional interaction energy is

$$V_i = \frac{1}{2}\sum_j \left(v_{ij,ij} + v_{i\bar{j},i\bar{j}}\right) = A\bar{v}.$$

Here the j summation runs over all occupied orbitals except i and we have defined an average interaction energy $\bar{v}$ in the last equality. We next add another particle to the system in orbital $\bar{i}$, giving an additional interaction energy, $V_i + v_{i\bar{i},i\bar{i}}$. Then $\Delta_o^{(3)}$ is given by half the difference,

$$\Delta_o^{(3)} = -v_{i\bar{i},i\bar{i}}/2 \qquad (6)$$

Adding a third particle gives an additional interaction energy of $(A+2)\bar{v}$. This can be used to obtain the following estimate for $\Delta_e^{(3)}$

$$\Delta_e^{(3)} = \bar{v} - v_{i\bar{i},i\bar{i}}/2. \qquad (7)$$

For the particle-particle interaction matrix elements associated with the time-odd contribution we use the same argument as with the pairing matrix elements G. This leads to the expectation that the average matrix elements embodied in the energies $\bar{v}$ and $v_{i\bar{i},i\bar{i}}$ also would have an A^{-1} dependence. The formulas Eq. (6) and (7) for the time-odd contribution were derived assuming that the orbital occupancies are zero or one, but the formulas remain valid in the presence of pairing in the nonblocked orbitals, as was the case for the single-particle contribution.

III. EXAMINING THE EXPERIMENTAL DATA

We now examine the experimental data on the OES, fitting it to various parametrizations. The data sets are defined with the same criteria used in ref. [18], using the Audi 2003 mass table [6]. We only include nuclei for which the experimental error on the binding energy is less than 200 keV, and make a further selection on the experimental data to avoid special binding effects not related to the mechanisms we have discussed. We drop nuclei with $N = Z$ because of their Wigner energy [13, 14] contribution. We also drop odd-odd nuclei which have an additional neutron-proton pairing [15, 16]. Finally, to isolate isospin dependencies, we require that the nuclei have positive isospin ($N > Z$). The sizes of the resulting data sets are given in Table II.

For each of the data sets we fit the OES with the following fitting functions:

i) A constant c_0. This is the naive BCS form, and sets the scale for any improvements of the phenomenology.

ii) The one-term, two-parameter function $c_\alpha A^{-\alpha}$ with prefactor c_α and exponent α which provides the minimum rms deviation. This shows the best one can do with two parameters, irrespective of justification.

iii) The two-term expression $c_1 + c_2/A$. The constant c_1 represents the BCS correlation energy, assumed independent of A, and the term c_2/A^{-1} represents interaction and single-particle contributions. We use additional subscripts o, e and n, p to distinguish the different OES measures.

The rms residuals of each of the four OES's with each of the three fit functions are shown in Table II. We also show the fit parameters for fits i) and iii).

TABLE II: Fits to the OES. Column 2 reports the size of each data set. Columns 3-5 show the rms residuals for the three fit functions discussed in the text. Columns 6-8 gives the fit parameters for models i) and ii). Units are MeV.

Data set		rms residual			fit parameters		
OES	Size	i	ii	iii	c_0	c_1	c_2
$\Delta^{(3)}_{on}$	443	0.313	0.254	0.270	1.04	0.82	24.
$\Delta^{(3)}_{en}$	442	0.420	0.278	0.308	1.32	0.94	41.
$\Delta^{(3)}_{op}$	418	0.275	0.220	0.231	0.96	0.75	25.
$\Delta^{(3)}_{ep}$	407	0.455	0.245	0.270	1.64	1.11	59.

A. Quality of fits

Let us first examine the quality of the fits. The simplest, just a constant, has an rms residual of about 0.3 MeV for the odd OES and 0.45 for the even OES measure. The residuals are decreased substantially, by up to 46%, going to the power law fit, model ii). Model iii) with two terms decreases the rms residual up to 41% and are almost competitive with model ii). In view of its better theoretical justification, we would advocate using it instead of the power-law fit. We note that the rms residual is larger for the even OES than for the odd one. This already suggests that shell fluctuations associated with the single-particle mechanism may be stronger than those affecting the time-odd contribution.

B. Neutron fit parameters

We now examine what information can be extracted from the fit parameters that we have obtained in model iii). Examining the neutron OES, we first note that the constant terms in the even and odd OES are close to each other; the ratio of the difference to the sum is $0.06/0.88 \approx 7\%$. Since the BCS is the only A-independent contribution, and it is common to both the even and the odd OES, the near-equality is just what we expect. Comparing the values to the one-term constant $c_0 \approx 1.0 - 1.3$, we see that the assigned BCS pairing represents only $\sim 75\%$ of the total on average.

The coefficients c_2, which we associate with the mean-field mechanisms, are quite different in the even and odd OES. That is also anticipated, since the two mechanisms we discussed affect them differently. From the coefficients c_{2o}, c_{2e} and an assumed single-particle contribution according to Eq. (3), we can extract average values for matrix elements in the time-odd contribution. These values are:

$$v_{i\bar{i},i\bar{i}} \approx -49 \text{ MeV}; \quad \bar{v} \approx -30 \,\text{MeV} \tag{8}$$

The signs and relative magnitudes are as expected for a basic NN interaction is attractive and short-ranged. For such interactions, the exchange contribution is large and attractive for $v_{i\bar{i},i\bar{i}}$ but not for $\bar{v}$. However, we cannot expect to extract reliable values from this simple approach for reasons already mentioned.

It is useful at this point to average the even and odd OES to emphasize the BCS correlation contribution and to look at the differences as well which will emphasize the mean field contribution. We define parameters

$c_{k\pm} = (c_{ko} \pm c_{ke})/2$ and show the fits in this form in Table III. The entries for the averages show again the relative importance of the mechanisms. The two terms give equal contribution at mass A satisfying $c_{1+} = c_{2+}/A$, giving $A \sim 40$ as the dividing point between light nuclei dominated by non-BCS pairing and heavier nuclei dominated by BCS pairing. We have already remarked that c_{1-} is small, as expected from a BCS pairing mechanism. The c_{k-} are essentially determined by the curvature of the binding energy surface in the two directions, along the Z axis for c_{k-p} and the N axis for c_{k-n}. In the liquid drop model, this curvature is mostly due to the Coulomb and symmetry terms in the formula. The curvature can be largely fit with the c_{2-}, as expected from the functional form of the symmetry term, $\sim (N-Z)^2/A$. The Coulomb is different, however, as we discuss below.

TABLE III: Averages and differences of the OES parameters, $c_{k\pm} = (c_{ko} \pm c_{ke})/2$. Columns 2-3 from the fit *iii*) shown in Table II. In the last row, the proton OES has been adjusted by subtracting the Coulomb interaction as discussed in the text. Units are MeV.

Parameter	$c_{1\pm}$	$c_{2\pm}$
c_{k+n}	0.88	33.
c_{k+p}	0.93	42.
c_{k-n}	0.06	8.
c_{k-p}	0.18	17.
c^*_{k-p}	0.10	14.

C. Proton fit parameters

We now turn to the proton OES. We first note that the c_{1+} has a slightly larger value than is found for the neutrons. It is tempting to interpret this as evidence for a stronger BCS pairing correlation energy for protons. There is of course additional physics associated with the mean-field aspects of the Coulomb interaction, but that affects only the difference coefficient c_{i-p}. From Table III we see that the c_{i-} parameters are not identical for neutrons and protons. The liquid-drop Coulomb energy, proportional to $Z^2/A^{1/3}$, gives rise to contributions to $\Delta^{(3)}_{op}$ or $\Delta^{(3)}_{ep}$ that have a very flat dependence on A. Parametrizing it according to model *iii*) gives Coulomb contributions $c_{i+p} \approx 0$ and $c_{1-p} \approx 0.08$ MeV ; $c_{2-p} \approx 3.$ MeV. In the bottom row, we subtract this contribution from the proton parameters. One sees that c_{1-p} is reduced to a value c^*_{1-p} much closer to the neutron value, c_{1-n}.

IV. SUMMARY AND CONCLUSIONS

The odd-even staggering of the binding energy depends on several effects. While a simple inverse power dependence can fit the general trends with mass number A, theory suggests different dependencies for the various terms. We have argued that three of the important contributions are single-particle energy spacing, BCS pairing, and particle-particle interactions, and that their A-dependence is given by A^{-1} for the single-particle energy contribution, A^0, i.e., constant, for BCS pairing, and A^{-1} for contributions from diagonal orbital interactions. A fit to the OES obtained from experimental masses indicates a significant improvement in the rms when both A^{-1} and constant terms are included. The rms values for fits with these two-term forms are slightly larger than for the values for the single inverse power form with an adjusted exponent. While both of these involve two free parameters the latter has no obvious theoretical basis, while the former does.

The results for the constant in the fit show that an A-independent BCS pairing requires on the order of 25% contribution from single-particle and time-odd interactions to the total average OES. The part left, attributable to BCS pairing, is slightly larger for protons than neutrons. This division implies that mean-field effects are more important than BCS pairing in light nuclei ($A <\sim 40$) and vice versa for heavy nuclei. Furthermore the diagonal Coulomb interaction is visible in the extract constants and is consistent with the liquid drop formula. The $1/A$ contributions can associated with the mechanisms of Table I, and a values for the interaction energies can be extracted. However, this part of the analysis is more speculative, in view the additional assumptions that must be introduced.

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